Final Report

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Tin-based IV-IV heterostructures by using Molecular Beam Epitaxy

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Highlights

The indirect nature of the fundamental energy gap in the elemental semiconductors Si and Ge prevents the use of these materials and their alloys in laser devices. The objective of the program is to fabricate Sn-based IV-IV compounds for finding direct bandgap material. Different material systems have been grown including GeSn on Ge wafer, SiGeSn on Si wafer etc. In the report, we present the results on the material system GeSn/Ge, covering from the growth, characterization, and optical measurement. Experimental evidences on pseudomorphic growth of thick $Ge_{1-x}Sn_x$ film for Sn composition up to 10% and the direct optical transition are presented. As a collaborated effort between NTU, UMass Boston, and AFRL at Hanscom, USA, we have also performed the designing of GeSn/Ge laser. In the next stage, we will forward to the fabrication of the designed structures. This report summarizes our (1) accomplishments, (2) future direction of work, and (3) publications produced as a result of this project.

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14. ABSTRACT
This is the final report of a project to fabricate tin-based IV-IV semiconductor compounds for obtaining direct bandgap material.

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(1) Accomplishments

In the conventional approach, Sn-based IV-IV compounds are mostly grown by the technique of Chemical Vapor Deposition (CVD). Different from the conventional approach, in this project, the Sn-based IV-IV compounds are fabricated by Molecular Beam Epitaxy (MBE). The technique affords flexibility in the growth of the materials system, whereby conditions such as growth temperature, etc., can be varied over a wide range. Different Sn-based IV-IV compounds are fabricated such as GeSn on Ge wafer, SiGeSn on Si wafer etc. In this report, we present the results on the material system of GeSn/Ge which we have completed a systematic investigation and direct optical transition is obtained. It is organized as three sections: (a) growth of GeSn [1-3], (b) characterization of the structure, (c) optical measurement, and (d) Design of GeSn/Ge laser.

(a) Growth of GeSn/Ge

By employing several proposed techniques, several key issues affecting the growth of the alloy and its heterostructure have been resolved. (α-Sn segregates during the growth of GeSn film and the misfit dislocations develop at GeSn/Ge interface as due to the large lattice mismatch between Sn and the Ge wafer.) A series of $Ge_{1-x}Sn_x$ films with various Sn compositions up to 30% and thickness of 30 nm was grown. From the analysis of Cross-sectional transmission electron microscope (XTEM) and Energy-Dispersive x-ray (EDS), for Sn composition $\leqq$ 10%, it shows that: (i) the $Ge_{1-x}Sn_x$ films are misfit dislocation free in the XTEM, and (ii) Sn is uniformly distributed in the $Ge_{1-x}Sn_x$ films. For Sn composition $\geqq$ 10%, the $Ge_{1-x}Sn_x$ films is not alloying with defects. All these film are thick above the predicted critical thickness which is required for the laser structure. To our best knowledge, thes defect free thick films is the first report in the literature.

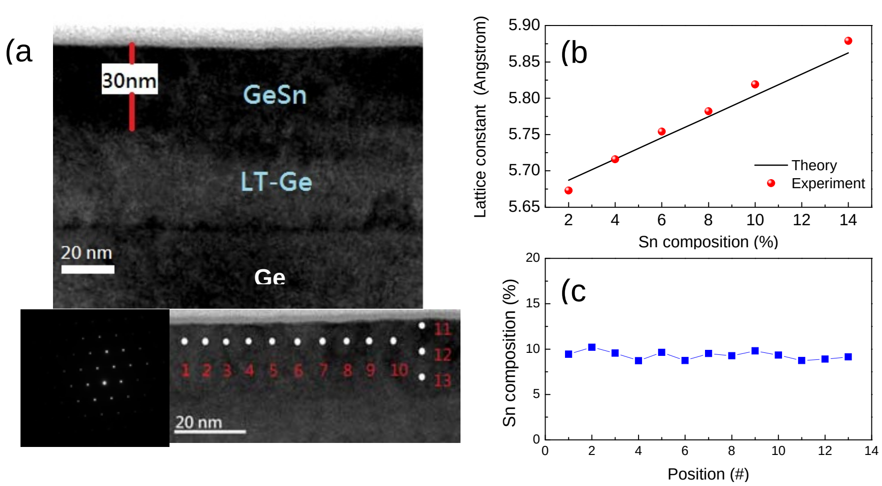

Fig. 1: (a) XTEM imagine of GeSn on Ge with the XRD, showing a single-crystal structure. (b) The lattice constant of GeSn film on Ge increases with the composition of Sn. (c) Position-dependent Sn composition of the GeSn, indicating Sn is uniformly distributed without segregation.

(b) Characterization of the structure

Various measurements have been performed to characterize these samples, including XTEM, EDS, high resolution X-ray, Raman spectroscopy, etc. The data of XTEM, EDS is depicted in Fig. 1. From high resolution X-ray, Raman spectroscopy, it shows that, these films are pseudomorphic with fully strained. Part of the results is presented in the last report and we will not present here.

(c) Optical measurement for probing the direct bandgap

Fourier transform infrared spectroscopy (FTIR) is employed for probing the bandgap of the GeSn film. The measurement is arranged in the setup with multi-reflection. A schematic diagram of the setup is plotted in fig. 2.

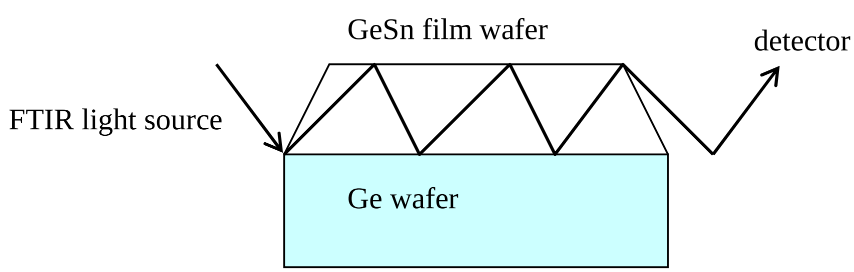

Fig. 2. Experimental setup for the FTIR absorption measurement.

The absorption spectrum of $Ge_{0.98}Sn_{0.02}$ film together with bulk Ge is shown in fig. 3. In comparison with bulk Ge, clearly, the absorption edge of the film shifts to lower energy. The spectrum is characterized by two features as marked by solid and dotted arrow lines. The two features locate at around 0.68 eV and 0.55 eV associated with the absorption originated from indirect and direct optical transitions. The value of the absorption is roughly the same as the theoretical value of 0.69 and 0.56 eV.

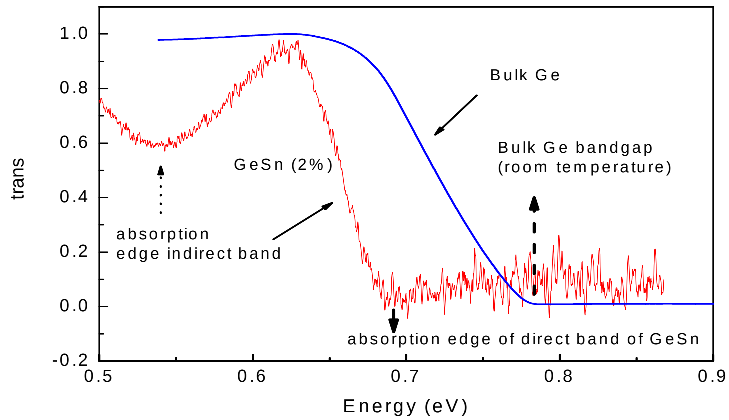

Fig. 3. Absorption spectrum of $Ge_{0.98}Sn_{0.02}$ films together with bulk Ge showing the indirect and direct optical transitions.

(d) Design of GeSn/Ge laser

We have also proposed two lattice-matched laser structures using GeSn as active layers and GeSiSn as barriers. One has a double heterostructure (DH) and another multiple quantum well (MQW) structure. The DH laser design is relatively easy to grow but only operates at low temperatures according our simulation [4], the MQW design, on the other hand, can potentially operate up to room temperature [5]. Lasing wavelength can be tuned from near to mid infrared with the Sn composition. On the implementation side, we have started to run growth of GeSn alloys with various compositions on Si substrates using MBE. While there are challenges in obtaining GeSn and GeSiSn layers with uniform compositions and of sufficiently low defects for device implementation, we have made progress over the past year and expect to continue this effort in the next proposal. Several cycles of laser designs, structure growth, device processing, and characterization will be necessary given the degree of complexity of this project. Laser designs will be refined with the material parameters obtained from the characterization of the actual structures grown on Si substrates, which in turn will guide the material and structure development and subsequent device processing.

(2) Future work

We have successfully overcome the technical issues of the growth of the material system of GeSn/Ge by employing MBE. Pseudomorphic growth of thick $Ge_{1-x}Sn_x$ film with uniform Sn distribution for Sn composition up to 10 % is demonstrated (Fig. 1). The thickness of these films is thicker than the critical film which is required for the laser structure. FTIR measurement reveals both indirect and direct optical transitions. In the next stage, we like to trace the bandgap of samples with different Sn compositions to establish the exact Sn composition of the crossover indirect-to-direct transition. This will enable us to draw a conclusive evidence for GeSn/Ge heterostructure with direct bandgap for GeSn/Ge optical emitter.

(3) Publications

[1] Local intermixing on Ge/Si heterostructures at low temperature growth, H. H. Cheng, W. P. Huang, V.I. Mashanov, and G. Sun J. Appl. Phys. 108, 044314 (2010). Selected paper by American Institute of Physics and the American Physical Society. Published by Virtual Journal of Nanoscale Science & Technology, http://www.vjnano.org, September 6, (2010).

[2] Pseudomorphic growth of Ge1-xSnx thick film at low temperature, submitted to APL.

[3] Formation of Ge-Sn nanodots on Si(100) surfaces by molecular beam epitaxy, Nanoscale Research Letters, publication date 12 January (2011).

[4] G. Sun, R. A. Soref, and H. H. Cheng, “Design of an electrically pumped SiGeSn/GeSn/SiGeSn double-heterostructure mid-infrared laser,” *J. Appl. Phys.* **108**, 033107 (2010).

[5] G. Sun, R. A. Soref, and H. H. Cheng, “Design of a Si-based lattice-matched room-temperature GeSn/GeSiSn multi-quantum-well mid-infrared laser diode.” Opt. Express 18, 19957-19965 (2010).